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Conserving approximations in nonequilibrium green function theory

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Stellingen
behorende bij het proefschrift
Conserving Approximations in
Nonequilibrium Green Function Theory
van
Adrian Stan
Groningen, 10 juni 2008

1. Total energies, ionization potentials and two-electron removal energies, obtained with our partially self-consistent GW approximation (*i.e.* the GW_{fc} approximation), are in very good agreement with fully self-consistent GW results, while requiring only a fraction of the computational cost.¹

Chapter 4 of this thesis

2. Fully self-consistent and partially self-consistent schemes provide ionization energies of similar quality as the G_0W_0 values, when calculated within the Extended Koopmans Theorem, but yield better total energies and energy differences than G_0W_0 calculated using the Galitskii-Migdal formula.¹

Chapter 3 of this thesis

3. [...] the Kadanoff-Baym equations can be used as a practical method to calculate the nonequilibrium properties of a wide variety of many-body quantum systems, ranging from atoms and molecules to quantum dots and quantum wells.

Chapter 5 of this thesis

4. Any Ξ -derivable theory is also Φ -derivable and therefore respects the conservation laws.

Chapter 7 of this thesis

5. Due to nonlinearity of the Kadanoff-Baym equations, the existence of bi-stable solutions and hence different steady states, may be possible.

Chapter 6 of this thesis

6. A *physica ex machina*² approach renders the scientific method as no more than a simple task to obtain numbers. It is too often forgotten that without understanding the path that lead to a result, the interpretation is meaningless.

7. Without a careful comprehension of the wellsprings of the claimed environmental threats, substituting the fossil fuel industry with any other type of industry, e.g., solar, hydrogen based, etc., will not solve the possible environmental issues. It will just replace them with similar ones.

8. For nothing but egalitarian reasons, the *Rijksuniversiteit* Groningen should instate a James Watson & Francis Crick fellowship, next to the Rosalind Franklin fellowship.

¹This statement refers to the calculations on small atoms and diatomic molecules presented in this thesis.

²Since at the time of publication of this thesis, a bibliographic search for the exact syntax "physica ex machina" returned no results, I use it here to single out a computational approach in the absence of a careful understanding of the method used and hence lacking a lucid interpretation. I translate this syntax as "physics from the machine" and I imply an allegorical relation with the expression "deus ex machina" as used in Horace's *Ars Poetica*. This statement is also meant to be generalized beyond its present connection to the field of physics.

